

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.18e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.31e-01

Confidence level: 3.27e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>p,p'-DDE</div> <div>Measured: 4.46e-11</div> <div>Predicted: 2.89e-06</div>	<div>Image not found</div> <div>Furalaxyl</div> <div>Measured: 1.13e-06</div> <div>Predicted: 3.22e-07</div>	<div>Image not found</div> <div>Sulcotrione</div> <div>Measured: 1.73e-08</div> <div>Predicted: 2.68e-08</div>
<div>Image not found</div> <div>Triacontane</div> <div>Measured: 2.40e-06</div> <div>Predicted: 8.27e-11</div>	<div>Image not found</div> <div>Oxalic acid</div> <div>Measured: 1.57e-10</div> <div>Predicted: 3.33e-04</div>	